First-Principles Simulations of 1 + 1D Quantum Field Theories at $\theta = \pi$ and Spin Chains

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We present a lattice study of a 2-flavor U(1) gauge-Higgs model quantum field theory with a topological term at $\theta = \pi$. Such studies are prohibitively costly in the standard lattice formulation due to the sign problem. Using a novel discretization of the model, along with an exact lattice dualization, we overcome the sign problem and reliably simulate such systems. Our work provides the first *ab initio* demonstration that the model is in the spin-chain universality class, and demonstrates the power of the new approach to U (1) gauge theories.

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Quantum field theories with θ terms are of immense interest, both in high energy as well as condensed matter physics. The θ angle is an example of a purely quantum deformation, which is inconsequential for the classical motion of the system. Yet the presence of the θ term can dramatically change a quantum system. A textbook example of a θ term is the motion of a particle on a ring in the presence of a magnetic flux. Classically the motion is undisturbed as the magnetic field is zero everywhere along the path of the particle. Still the quantum system can feel the magnetic field through the Aharonov-Bohm effect, reshuffling the spectrum back onto itself as the magnetic flux is increased to the unit flux quantum. The θ term in the path-integral description precisely corresponds to the magnetic flux, normalized such that $\theta = 2\pi$ corresponds to the unit flux quantum.

In quantum chromodynamics the possibility to write a θ term is the basis of the strong CP problem, which is among the most important problems of modern high-energy physics. More relevant for this work is that in the effective description of antiferromagnetic (AFM) spin chains θ terms may arise due to the Berry phases in the path-integral quantization of spin, as first noted by Haldane [1]. The observation that integer and half-integer spin chains are distinguished in the effective field theory description by the value of the θ parameter, $\theta = 0$ and $\theta = \pi$, respectively, is the basis of Haldane's conjecture.

Haldane's work, along with the integrability of the $S = 1/2$ Heisenberg model, the idea of non-Abelian bosonization [2] and the theoretical tractability of the Wess-Zumino-Witten (WZW) theories [3,4], gives a compelling self-consistent picture of the $\theta = \pi$ Abelian field theory, which we will review below. Yet very little is understood from first principle computer simulations. The reason is that the introduction of the θ term gives rise to a complex weight in the conventional formulation of the path integral, which prohibits efficient Monte Carlo sampling. Recently, we have proposed a solution to this sign problem relevant for such systems. The approach relies on the reformulation and dualization of U(1) lattice gauge theory in two dimensions [5], that was generalized to higher dimensions by two of us in Ref. [6]. Here we apply these ideas to a 2-flavor U(1) gauge-Higgs model, relevant for spin chains. Using first principle numerical calculations we, for the first time, confirm the theoretical picture that arises indirectly by other reasoning. At the same time the consistency gives credence to our novel approach to U (1) lattice gauge theories, which have applications also in higher-dimensional spin systems, most notably to the yet unsettled deconfined quantum criticality in $(2+1)$D antiferromagnets (see, e.g., Refs. [7–10] and references therein). On the other hand, our formulation may also have interesting implications for fundamental aspects of electrodynamics on the lattice, including electric magnetic duality, and the possible existence of a continuum limit [6] contradicting the general lore. The success of our methods demonstrated here in $(1+1)$D are an important step towards a better understanding of U(1) gauge theories and their interdisciplinary significance.

The model and its connection to spin chains.—The model we study is the 2-flavor Abelian gauge-Higgs model described by the Euclidean Lagrangian

$$\mathcal{L} = \frac{1}{4e^2} F_{\mu\nu} F^{\mu\nu} + \frac{i\theta}{2\pi} F_{12} + (D_\mu \Phi)^\dagger (D_\mu \Phi) + m^2 \Phi^\dagger \Phi + \lambda (\Phi^\dagger \Phi)^2, \qquad (1)$$

where $\mu = 1, 2$ is the space-time index, $\Phi = (\phi_1, \phi_2)^T$ is an SU(2) scalar doublet. $F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$ and $D_\mu = \partial_\mu + iA_\mu$, with A_μ the U(1) gauge field. We will view the above theory in the spirit of an effective theory, so that the Lagrangian should be supplemented with a UV cutoff Λ. A transformation $\Phi \to U\Phi$ where U is an SU(2) unitary matrix is a symmetry of the Lagrangian. However, the $\mathbb{Z}_2$ center symmetry of SU(2) acting as $\Phi \to -\Phi$ is a subgroup of the U(1) gauge symmetry $\Phi(x) \to e^{i\varphi(x)}\Phi(x)$, so the global symmetry is $SU(2)/\mathbb{Z}_2 \cong SO(3)$ instead. Moreover the system has a charge conjugation symmetry $\mathcal{C}$ which takes $\Phi \to \Phi^*$ and $A_\mu \to -A_\mu$, when $\theta = 0$ or π, which, together with SO(3) forms the symmetry group O(3).

U(1) gauge theories in two dimensions are natural candidates for spin-1/2 AFM spin chains. The history of the connection of model (1) to spin chains is a long one, with some more recent developments involving anomalies, which we briefly review here.

Consider first the limit (It is conventional in high-energy literature to label the coupling in the Lagrangian as m^2, such that when m^2 is positive, m is the tree-level mass of the Φ excitations.) $-m^2 \ll \Lambda^2$, such that the classical potential is minimized at the value $\Phi = \Phi_0 = u\sqrt{|m^2|/(2\lambda)}$, where u is a two-component unit vector. Writing $\Phi(x) = u(x)\sqrt{|m^2|/(2\lambda)}$, the limit $-m^2 \ll \Lambda^2$ effectively sets $u^\dagger u = 1$ and the model reduces to the weakly coupled $CP(1)$ nonlinear sigma model (NLS), which is equivalent to the $O(3)$ NLS model [To be precise, the $CP(1)$ model has no kinetic term for the gauge field. However, the kinetic term is irrelevant (i.e., the coupling e is relevant), so its presence is not expected to change the behavior. Alternatively, we can think of the model with a nonzero kinetic term as the RG iterated $CP(1)$ model, where the kinetic term is generated along the RG flow [11].].

The opposite limit of the model (1), where m^2 is large and positive is exactly computable, as the Φ field is massive and can be integrated out. The result is a pure gauge theory at $\theta = \pi$, which is exactly solvable and has a double vacuum degeneracy due to the $\mathcal{C}$-symmetry breaking.

On the other hand Haldane has shown that the SU(2) Heisenberg spin-chain in the spin S representation is equivalent to the weakly coupled O(3) model in the large S limit [1], where the θ angle is given by $\theta = 2\pi S \bmod 2\pi$ for translationally invariant systems, indicating that the integer and half-integer SU(2) spin chains fall into separate universality classes. This is nicely consistent with the Lieb-Shultz-Mattis (LSM) theorem [The LSM theorem states that an SO(3) and translationally invariant antiferromagnetic spin chain is either gapless, or breaks translation symmetry spontaneously.] [12,13], which, along with the integrability of the $S = 1/2$ Heisenberg spin chain, gives credence to the conjecture that the O(3) model at $\theta = \pi$ is critical (see also Ref. [14]). This in turn leads to the plausible conjecture that all half-integer Heisenberg spin chains are critical. Furthermore, the $\theta = \pi$ $O(3)$ model, as well as its cousin (1), are subject to a variety of anomaly matching constraints [15–19]—which should be viewed as LSM-like theorems.

Lattice theory and duality.—The usual lattice discretization uses U(1) valued phases on links. When considering the 2D theory with the θ term, it is, however, useful to instead define $\mathbb{R}$-valued gauge fields A_l on links l, supplemented by integer-valued variables n_p living on the plaquettes p, with gauge action

$$S_G[A,n] = \sum_p \frac{\beta}{2}(F_p + 2\pi n_p)^2 + i\theta \sum_p n_p, \qquad (2)$$

where $\beta = 1/2e^2$ is the inverse gauge coupling, and F_p the discretized version of the field strength. Apart from the θ term, the above action is the well-known Villain discretization of U(1) lattice gauge theory [20], while the θ term was introduced in Refs. [5,6] (The n_p play the role of a discrete 2-form gauge field which allows the values of the A_l to be restricted to $[-\pi,\pi]$. Moreover, similar reasoning can be used to make a connection [6] with the geometric definition of the topological charge [21].). Using Poisson resummation it is possible to replace

$$\sum_{n_p\in\mathbb{Z}} e^{-\frac{\beta}{2}(F_p+2\pi n_p)^2 + i\theta n_p} \to \sum_{m_p\in\mathbb{Z}} e^{-\frac{1}{2\beta}(m_p+\frac{\theta}{2\pi})^2 + iF_p m_p}, \qquad (3)$$

such that the action is now linear in F_p. Integrating out the A_l after the appropriate "partial integration" imposes the constraint that for pure gauge theory m_p is constant on all plaquettes, with a remaining weight that is real and positive.

The matter sector of model (1) is described by an SU(2) bosonic (Higgs) doublet Φ on lattice sites x, with the action

$$S_H[\Phi,A] = \sum_x \Bigg[M\Phi_x^\dagger\Phi_x + \lambda(\Phi_x^\dagger\Phi_x)^2 - \sum_{\mu=1}^{2}(\Phi_x^\dagger e^{iA_{x,\mu}}\Phi_{x+\hat{\mu}} + \text{c.c.}) \Bigg], \qquad (4)$$

where $M = 4 + m^2$. In Eq. (4) we denote links l as (x,μ) and $A_{x,\mu}$ is a gauge field on a link rooted at x in the direction μ. The partition function with the above matter-action can be dualized to a sum over closed U(1) currents described by closed contours $\mathcal{C}$ built out of lattice links, which couple to the gauge field as $e^{i\sum_{l\in\mathcal{C}} A_l}$. After the insertion of such wordlines, A_l can be integrated out, causing m_p to jump at the worldlines by the amount of U(1) charge carried by the wordline. If the matter field in question is bosonic, as in Eq. (1), the statistical weight of the configurations is strictly positive, allowing for Monte Carlo simulations in the dual representation. Using suitable methods [22] we simulate the model (1), varying m^2 at fixed $\lambda = 0.5$ and $\beta = 3$. See Supplemental Material [23] for details.

Phase diagram and numerical results.—The LSM theorem states that if $O(2) \subset SO(3)$ spin and lattice translations are good symmetries of a half-integer spin chain, then either the spin chain is gapless, or gapped and degenerate. On the other hand, the field theory at $\theta = \pi$ has an analogous 't Hooft anomaly involving the charge-conjugation symmetry $\mathcal{C}$ and the spin symmetry SO(3), implying that either the $\mathcal{C}$ is broken or that the theory is gapless [15–19]. Both of these are nicely consistent with the limits of $m^2 \to \pm\infty$ we discussed above, and the critical to dimer transition of spin chains (see, e.g., Refs. [24–27]), provided that the translation symmetry is identified with the symmetry (The label $\mathcal{CF}$ is there to imply that the transformation is a combination of the $\mathbb{Z}_2$ flavor symmetry subgroup $\mathcal{F}: \Phi \to i\sigma^2\Phi$ and the $\mathcal{C}$ symmetry.) $\mathcal{CF}: \Phi \to i\sigma^2\Phi^*$, where σ^2 is the standard Pauli matrix.

It is natural to conjecture that the phase transition between the $m^2 \to \infty$, $\mathcal{C}$-broken phase to the $m^2 \to -\infty$, O(3) NLS phase is of the same nature as the phase transition between the dimerized phase of spin chains and the critical phase described by the $\mathrm{SU}(2)_1$ Wess-Zumino-Witten theory. One argument for this is that the $\mathrm{SU}(2)_1$ WZW theory can be deformed to the O(3) NLS model at $\theta = \pi$, but only with the use of irrelevant deformations, indicating that the O(3) NLS model at $\theta = \pi$ would like to flow to the WZW theory.

The picture above is compelling and largely a matter of textbooks by now (see, e.g., Ref. [28]). It does, however, rely on many assumptions, such as robustness of the critical WZW phase under large irrelevant deformations, the validity of the large S limit down to $S = 1/2$, etc. The development of a suitable formulation of a lattice model which can be simulated at $\theta \neq 0$, allows us for the first time to provide reliable *ab initio* data for the model (1), and to confirm the above picture (Some numerical experiments on NLS models were performed in Refs. [29–33], but as opposed to our approach their applicability is limited, and not easily generalizable to other interesting cases.).

To test whether the transition from the $m^2 \to \infty$, $\mathcal{C}$-broken phase to the $m^2 \to -\infty$ phase is of the same nature as the dimer to critical spin chain transition, we must discuss its universal properties. The relevant critical phase of the spin chains is the $\mathrm{SU}(2)_1$ WZW phase [34], which was checked by numerous simulations [27,35–38] and is consistent with the $S = 1/2$ integrable Heisenberg model [25]. The $\mathrm{SU}(2)_1$ WZW model has no relevant couplings preserving the symmetries of the spin chain [34], and thus the gapless phase is (believed to be) a fairly robust phase. A potential instability of the WZW phase lies in a marginal operator [25], with a coupling g_m, which is either marginally relevant or marginally irrelevant, depending on the sign, and it is this coupling that drives the transition from the WZW to the $\mathcal{C}$-broken phase. When $\theta \neq \pi$, a relevant operator with scaling dimension $x = 1/2$ and coupling $g_r \propto (\theta - \pi)$ will be present in the effective action [3,4,25]. This operator of course breaks the $\mathcal{C}$ symmetry (and translation symmetry of the spin chain). The RG equation for this coupling is

$$a\frac{dg_r}{da} = (2 - x)g_r = \frac{3}{2}g_r, \tag{5}$$

where a is a sliding cutoff (length) scale. At the transition point between the $\mathcal{C}$-broken and the WZW phase, $g_m = 0$ and the spin-Peierls mass gap opens up $M_{\mathrm{SP}} \propto g_r^{2/3}$. At finite volume L^2, the singular free energy density (The free energy density transforms under the RG flow with two parts. The first comes from integrating the short-distance degrees of freedom, while the second—so-called singular or homogeneous—part is due to the scale transformation. It is the second part that is relevant for the critical behavior; see, e.g., Ref. [39].) must be of the form

$$f = \frac{1}{L^2}F(g_r L^{3/2}). \tag{6}$$

This follows from the fact that in two dimensions the free energy density scales like the inverse correlation length squared, and that near $g_r = 0$ the dependence on g_r must be through the combination $M_{\mathrm{SP}}L$. For the susceptibility at $g_r = 0$ we thus find

$$\chi = \frac{\partial^2}{\partial g_r^2} f \Big|_{g_r=0} \propto L. \tag{7}$$

All of this is valid for $g_m = 0$, while logarithmic volume corrections need to be taken into account when $g_m \neq 0$ [25]. This means that if we plot χ/L for different volumes, as we vary m^2 in the model (1) there should be a point $(m^2)_c$ where the curves for different volumes intersect, provided that the $1/L$ corrections are sufficiently small (The definition of the topological susceptibility we use is shifted by an overall constant, which is a trivial shift in the dual representation that we employ.).

Figure 1(a) shows the numerical data for four volumes with linear dimension $L = 32$, 48, 64, and 80, and indeed one can clearly see a point where all curves intersect. The simulations were performed for m^2 in the interval $[-1.8, -1.5]$, varying m^2 in steps of 0.05. These Monte Carlo data were then used to obtain the curves in Fig. 1(a) using reweighted interpolation. The inlay in Fig. 1(a) shows an enlargement into the crossing region for which a separated reweighted interpolation with data from the three indicated points was generated. The four curves intersect at $(m^2)_c = -1.73(1)$ to within the specified accuracy, which gives our estimate of the transition point.

To confirm the nature of the phase transition, we need to derive the scaling form of the topological susceptibility in the presence of a nonzero coupling g_m. The RG equations for g_m and g_r are [25]

$$a\frac{dg_m}{da} = \pi b_m g_m^2, \qquad a\frac{dg_r}{da} = \left(\frac{3}{2} + 2\pi b_r g_m\right)g_r, \tag{8}$$

where the sign of g_m is chosen such that g_m is marginally relevant when positive (Note that this is the opposite

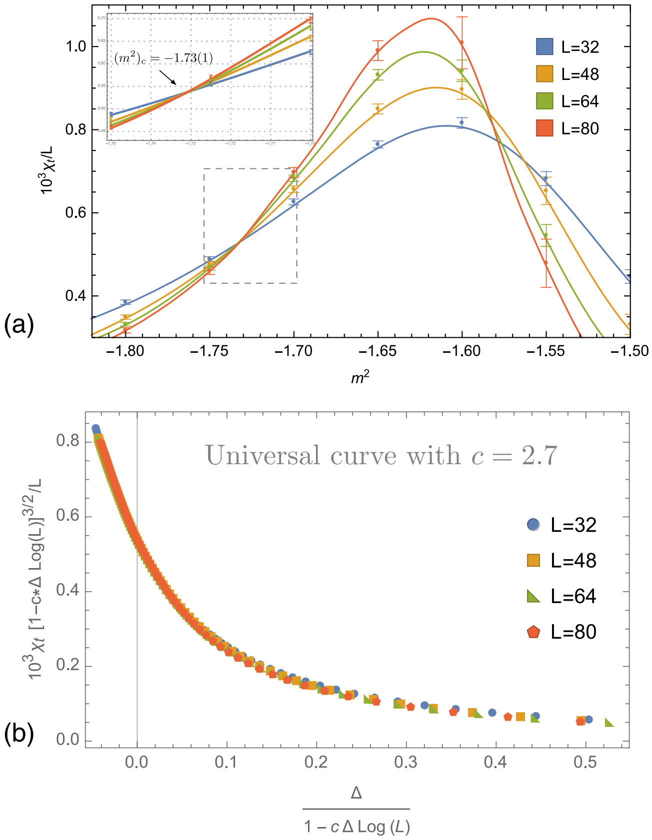

FIG. 1. Reweighted interpolation data for the topological susceptibility χ_t. (a) χ_t/L for various values of the linear dimension L of the system. All curves intersect well at the point $(m^2)_c = -1.73(1)$, which is consistent with the scaling of the $SU(2)_1$ WZW theory, at marginal coupling $g_m = 0$. The inlay show the interpolation data for the dashed region. (b) the same data obey the scaling form (9), for $c = 2.7$.

convention of that in Ref. [25].). The constants b_m and b_r are determined by the three-point functions [25], and depend on normalization of the two-point functions. Indeed, in the above RG equations we can always eliminate either b_r or b_m by redefining g_m. One can show that the free energy density at finite volume must be of the form

$$f = \frac{1}{L^2} F\left(\frac{\pi b_m g_m}{1 - \pi b_m g_m \log(L)}, \frac{g_r L^{3/2}}{(g_m)^{\frac{2b_r}{b_m}}}\right). \tag{9}$$

This result requires some discussion: Under an RG flow the UV cutoff changes as $a \to a' > a$, while the linear dimension L shrinks to $(a/a')L$, so that L can be thought of as changing under the RG flow as the correlation length or inverse mass gap. The overall factor of $1/L^2$ above accounts for the RG flow of the singular free energy density, so that the F function must be constant under the RG flow. For the bare couplings $g_m > 0$, $g_r = 0$, an exponentially small mass gap opens $\propto \exp[-(\pi b_m g_m)^{-1}]$, so the universal function F must

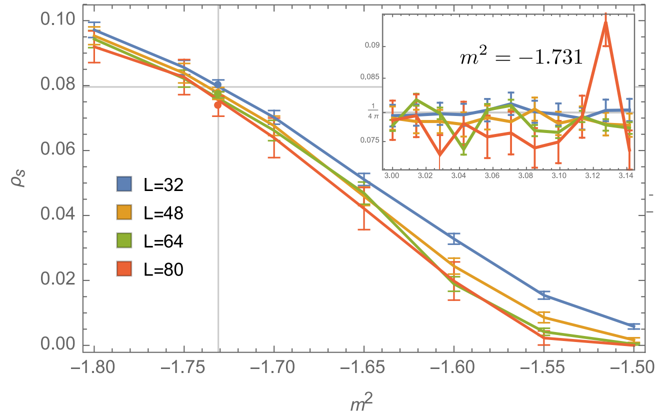

FIG. 2. Spin stiffness as a function of m^2. At the transition point $m^2 = (m^2)_c = -1.731$ (marked with a vertical line), where the marginal coupling $g_m = 0$ is expected to be zero, it shows good agreement with the universal value $\rho_s = 1/4\pi$ (horizontal line). The inlay shows the stiffness at the transition point for different values of θ between 3.0 and π.

depend on the combination $\exp[-(\pi b_m g_m)^{-1}]L$. The first argument of F in Eq. (9) is just the reciprocal of the logarithm of this combination. When $g_r \neq 0$ it is also straightforward to check that the 2nd argument in Eq. (9) is also RG invariant. The same is true for $g_m < 0$, so that Eq. (9) holds as long as g_m, g_r are sufficiently small.

Taking the second derivative of Eq. (9) with respect to g_r we find

$$\chi_t = \frac{L}{(1 - c\Delta \log L)^{\frac{4b_r}{b_m}}} X\left(\frac{\Delta}{1 - \Delta c \log(L)}\right), \tag{10}$$

where we set $g_m \propto \Delta = m^2 - (m^2)_c$, and introduced an undetermined coefficient c, and where X is some universal function.

We already remarked that $g_r \neq 0$ corresponds to a deviation of θ away from π, which induces a spin-Peierls transition, such that $(2b_r/b_m) = (3/4)$ [25], and the exponent in the prefactor of Eq. (10) is fixed. Figure 1(b) shows that the data indeed nicely follow the scaling form (10) for a choice of $c = 2.7$.

As an additional check, in Fig. 2 we show results of a calculation of the spin stiffness ρ_s, which measures the response of a system to a constant spatial gauge field A_1 for a U(1) subgroup of the SO(3) symmetry, i.e.,

$$\rho_s \equiv \frac{1}{L^2} \frac{\partial^2 \log Z}{\partial A_1^2}. \tag{11}$$

The $SU(2)_1$ WZW theory has a description in terms of a compact scalar field $\phi(x) \sim \phi(x) + 2\pi$, with Lagrangian [The model has only a manifest U(1) symmetry, but in fact the symmetry is $SU(2) \times SU(2)$ (see, e.g., Ref. [40]).]

$$\mathcal{L} = \frac{1}{4\pi}(\partial_\mu \phi)^2. \quad (12)$$

The corresponding spin stiffness can be explicitly calculated [23] and is given by [Note that this result is slightly subtle, as the naive expectation is that ρ_s is the same as 2 times the coefficient of the kinetic term in Eq. (12), but this is not the case here (see, e.g., Ref. [41]).] $\rho_s = 1/4\pi$.

In Fig. 2 we plot the stiffness for various volumes, and indicate the phase transition point (vertical line), as well as the stiffness $\rho_s = 1/4\pi$ for the $\mathrm{SU}(2)_1$ WZW model (horizontal line). As can be seen, exactly at the transition point the stiffness for all volumes is very close to the expected value. We have also computed the stiffness at the critical point for values of θ away from π and show the corresponding results in the inlay of Fig. 2.

Conclusion and future work.—We have presented Monte Carlo simulations of the lattice 2-flavor U(1) gauge-Higgs QFT model, with a topological angle θ. We were mostly interested in the value $\theta = \pi$, for which the model is supposed to be an effective description of a half-integral spin chain. Such spin chains with a full SO(3) spin symmetry can be in two phases: in the dimerized phase with a twofold degenerate gapped ground state, and in the critical $\mathrm{SU}(2)_1$ WZW phase. We have shown that the lattice discretization we proposed in Refs. [5,6], which has the correct symmetries and anomalies, gives rise to *ab initio* results consistent with the expected WZW or dimerized transition.

This not only complements decades of research on antiferromagnetic spin chains and their connections to QFTs with θ terms, but also shows the potential of the novel lattice formulation of Abelian gauge theories [5,6], which have applications not only to other interesting 2D models like the asymptotically free CP^{N-1} models, and flag-manifold sigma models related to $\mathrm{SU}(N)$ spin chains [19,42–44], but also for U(1) gauge theories in higher dimensions. Such formulations allow an enhanced control over monopoles in abelian gauge theories, which are relevant for higher-dimensional spin systems (e.g., for deconfined criticality of antiferromagnets in 2 spatial dimensions [7]) and the lattice theory of electromagnetism, where monopoles were thought to be an unavoidable curse on the lattice.

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